3-Amino-3-(naphthalen-1-yl)propanoic acid

100393-41-7 | DTXSID80377489

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.36e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.30e-01

Confidence level: 3.72e-01

Nearest Neighbors from the Training Set

Image not found
3-Amino-3-(naphthalen-1-yl)propanoic acid
Measured: 2.57e-02
Predicted: 1.36e-02

Image not found
Indole-3-butyric acid
Measured: 1.23e-03
Predicted: 1.38e-02

Image not found
Indole-3-acetic acid
Measured: 8.56e-03
Predicted: 1.59e-02

Image not found
6-Quinolinecarboxylic acid
Measured: 9.00e-01
Predicted: 7.26e-02

Image not found
Quinoline-5-carboxylic acid
Measured: 2.10e-03
Predicted: 7.19e-02